Optical effects in multiband conductors and superconductors

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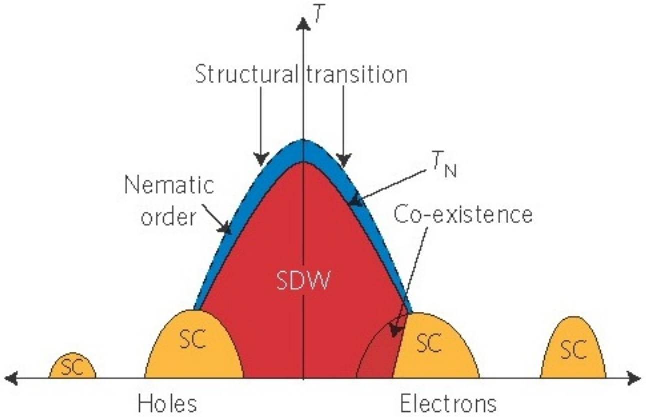
Outline



- Determination of optical properties
- Optical properties of metals and SC's
  - Drude model and Landau Fermi liquid (FL)
  - clean- and dirty-limit superconductors
- Iron-based superconductors: multiband materials
  - *e* and *h* pockets: "two-Drude" approach
  - $BaFe_2As_2$: metallic parent compound
    - magnetic/structural transition $\rightarrow$ FS reconstruction
    - collapse of scattering rate $\rightarrow$ Dirac-like cones
    - analogies in cuprates?
  - $FeTe_{0.55}Se_{0.45}$ (T_c=14 K) & $Ba_{0.6}K_{0.4}Fe_2As_2$ (T_c=39 K)
    - hidden FL and non-FL states
    - clean and dirty limit superconductors, etc.
- Summary

Complex optical properties

- Reflectance is complex: $\tilde{r} = \sqrt{R}e^{i\theta}, R = \tilde{r}\,\tilde{r}^*$
  - usually only *R* is measured
- Measure *R* over wide range, determine θ
  - Kramers-Kronig relation

$$\tilde{r} = \sqrt{R}e^{i\theta},\ \ln\tilde{r} = \tfrac{1}{2}\ln R + i\theta$$
$$\theta(\omega_0) = \frac{\omega_0}{\pi}\int_0^\infty \frac{\ln[R(\omega)] - \ln[R(\omega_0)]}{\omega_0^2 - \omega^2}d\omega$$

- From R, θ: $\tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2, \tilde{\sigma} = \sigma_1 + i\sigma_2$

$$\sigma_1(\omega) = 2\pi\,\omega\,\varepsilon_2 / Z_0\ (\Omega^{-1}\mathrm{cm}^{-1});\ \sigma_{dc} \equiv \sigma_1(\omega \to 0)$$

  - connection with transport
  - important self-consistency condition…
- Absolute value of *R* is critical…

CCH *et al*., Appl. Opt. **32**, 2976 (1993).

Drude metal & Landau Fermi liquid

- Drude model: no interactions

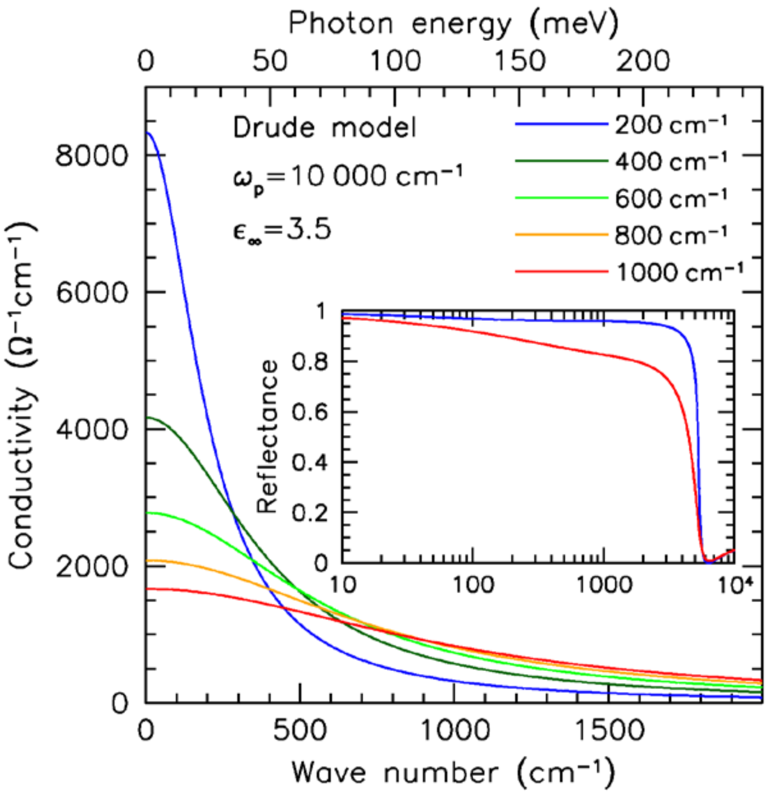
$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty - \frac{\omega_{p,D}^2}{\omega^2 - i\omega/\tau_D}, \quad \omega_{p,D}^2 = \frac{4\pi n e^2}{m^*}$$

$$\sigma_1(\omega) = \omega\varepsilon_2 / 60$$

- Conductivity: Lorentzian at ω=0
  - FWHM: $1/\tau_D$
- Scattering rate $1/\tau_D$ varies with T
  - no *a priori* T dependence
- Landau Fermi liquid: interactions

$$\frac{1}{\tau(\omega,T)} = \frac{1}{\tau_0} + A\left[(\hbar\omega)^2 + (2\pi k_B T)^2\right]$$

  - quadratic in T and ω



f-sum rule: $\int_0^\infty \sigma_1(\omega')\,d\omega' = \frac{\omega_p^2}{8}$

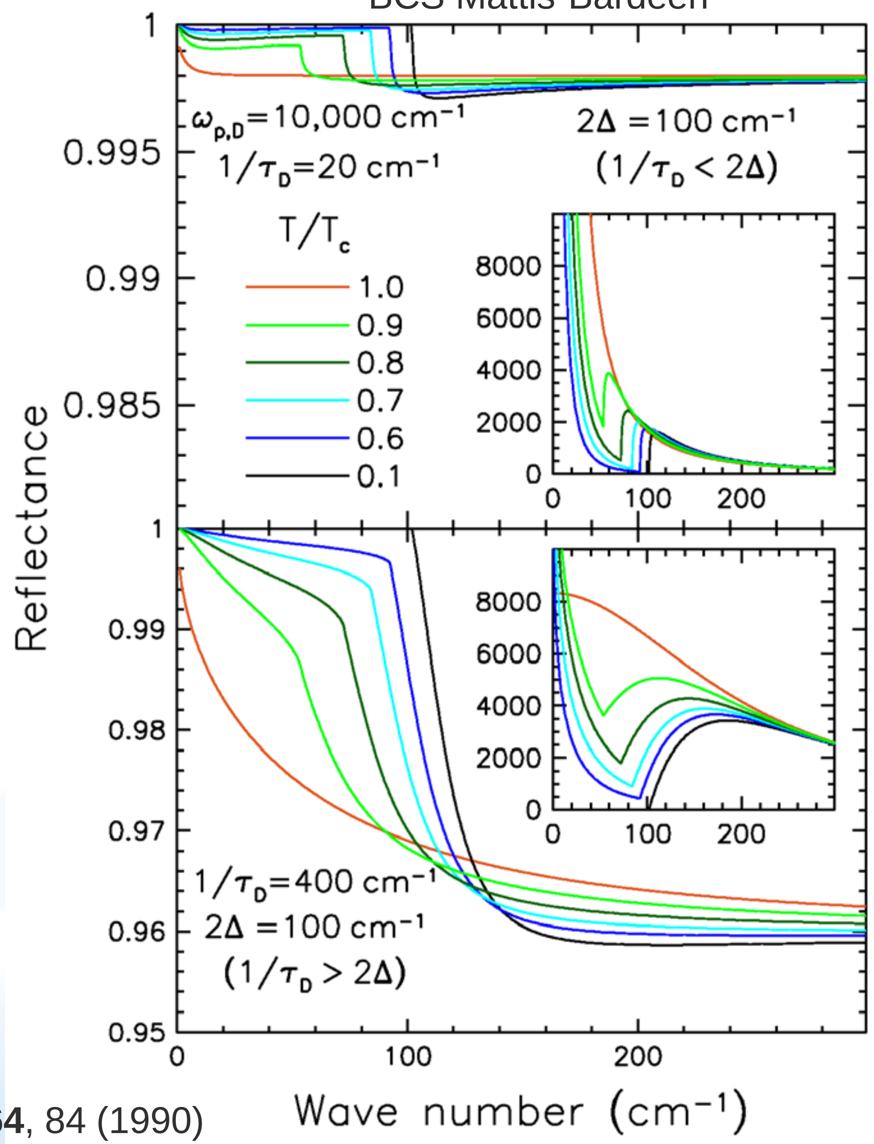
S. V. Dordevic and D. N. Basov, Ann. Phys. (Leipzig) **15**, 545 (2006)

Optical manifestation of SC gaps

- Normal state: Drude
- "Good" metal: *R* > 99.5%
  - $1/\tau_D < 2\Delta$
    - "clean limit"
  - SC gap is hard to see
- In a "bad" metal, optical signature of SC is clear
  - $1/\tau_D \sim 2\Delta$
    - "dirty limit"
  - large changes below T_c
  - missing spectral weight

$$N(\omega) = \int_{0^+}^{\omega} \sigma_1(\omega')\, d\omega'$$

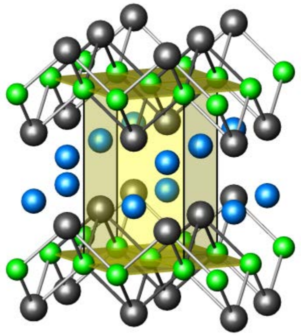
BCS Mattis-Bardeen

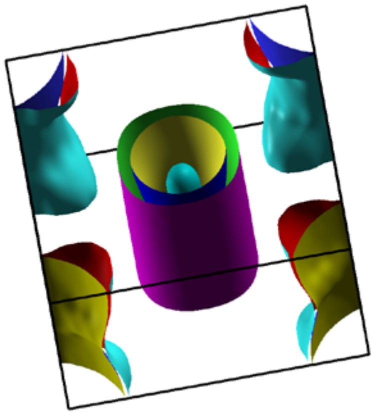


K. Kamarás *et al.*, Phys. Rev. Lett. **64**, 84 (1990)

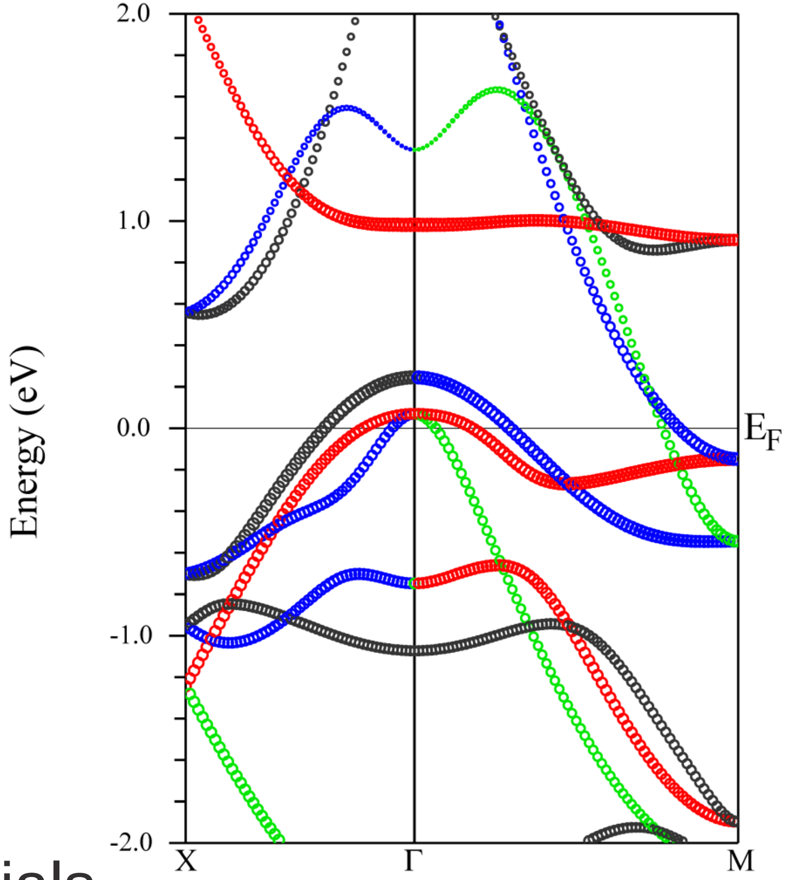
Iron-based superconductors

- Multiband materials, T_c's > 50 K
  - three hole-like bands at Γ
  - two electron-like bands at M
- Example: LiFeAs (WIEN2k/GGA)
  - RT tetragonal: P4/nmm (129)
    - relaxed geometry





Orbital character: Fe-*d*

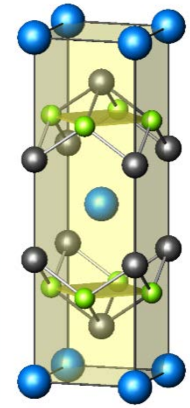


(d_{xy}, d_{xz}+d_{yz})

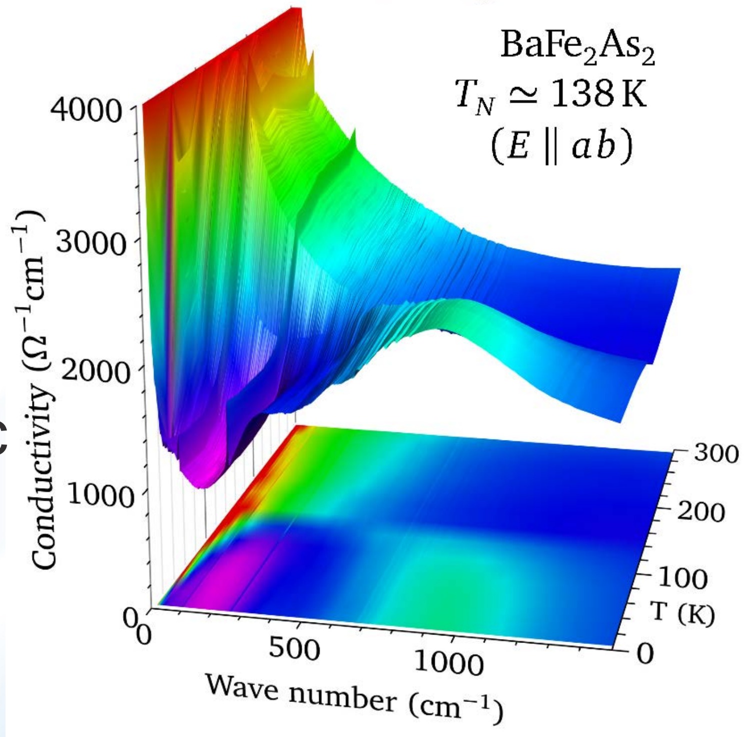
- Similar for most iron-based materials
  - uncorrelated, neglected spin-orbit, etc.

A. Subedi *et al.*, Phys. Rev. B **78**, 134514 (2008)

Parent material: $BaFe_2As_2$



- $BaFe_2As_2$
  - parent material for *e* and *h*-doped SC's
  - metallic (unlike cuprates)
- Structural and magnetic transition at T_N~138 K
  - tetragonal $\rightarrow$ orthorhombic
    - SDW-like transition
  - FS reconstruction, remains metallic
- Optical conductivity shows dramatic changes below T_N
  - transfer of spectral weight from low to high frequency
  - very narrow Drude component



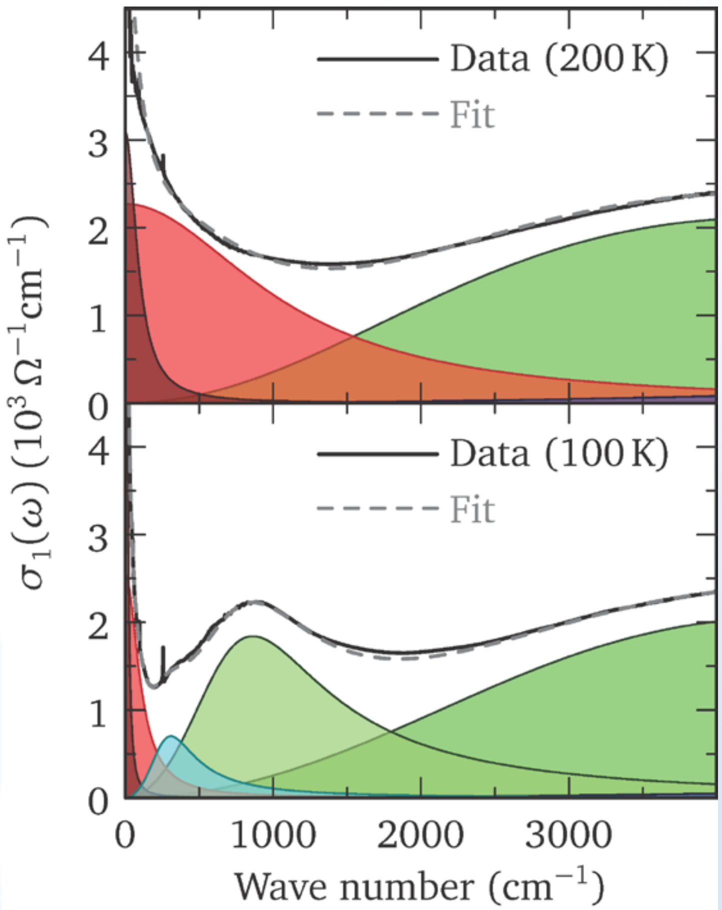
Two-Drude model

- Minimal description is a two-band system: "two-Drude" model
  - complex dielectric function

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty - \sum_{j=1}^{2} \frac{\omega_{p,j}^2}{\omega^2 + i\omega/\tau_j} + \sum_k \frac{\Omega_k^2}{\omega_k^2 - \omega^2 - i\omega\gamma_k}$$

$$\tilde{\sigma}(\omega) = \sigma_1 + i\sigma_2 = -2\pi i\omega\left[\tilde{\varepsilon}(\omega) - \varepsilon_\infty\right]/Z_0$$

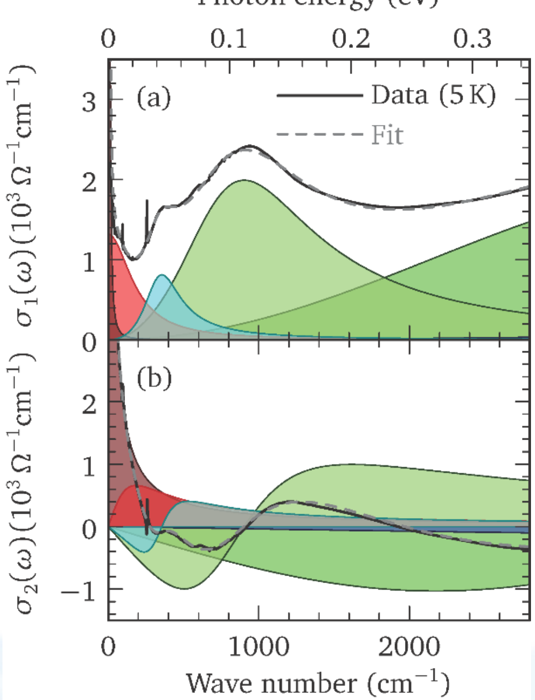
  - plasma frequencies: $\omega_{p,j}$
  - scattering rates: $1/\tau_j$
- Non-linear least-squares fit to both real and imaginary part of conductivity simultaneously
- Narrow and broad Drude terms…



D. Wu *et al.*, Phys. Rev. B **81**, 100512(R) (2010)
Y. M. Dai, CCH *et al.*, PRB **94**, 195142 (2016)

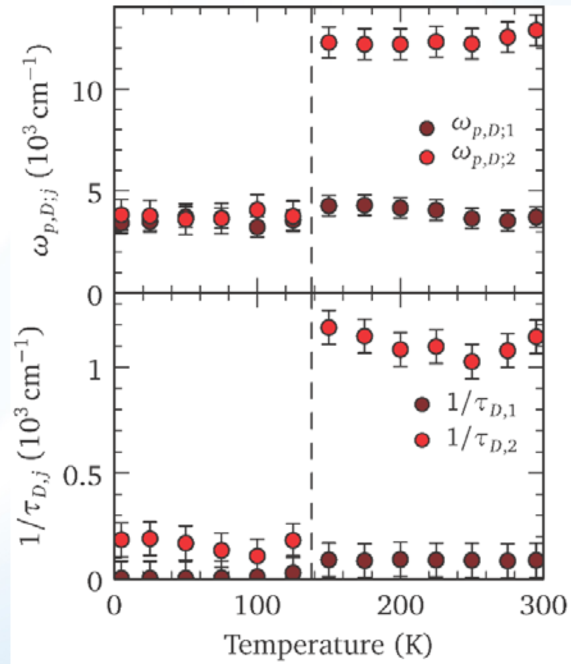
Fits to the optical conductivity

- $T > T_N$: little temperature dependence
- $T < T_N$: plasma frequencies, scattering rates decrease
  - $\omega_{p,D1} \cong 12900 \rightarrow 5100\ \mathrm{cm}^{-1}$; $\omega_{p,D2} \cong 4200 \rightarrow 3200\ \mathrm{cm}^{-1}$
  - $1/\tau_1 \cong 1200 \rightarrow 190\ \mathrm{cm}^{-1}$; $1/\tau_2 \cong 90 \rightarrow 3\ \mathrm{cm}^{-1}$



$$\sigma_{1,D}(\omega) = \frac{\sigma_0}{1+\omega^2\tau_D^2}$$

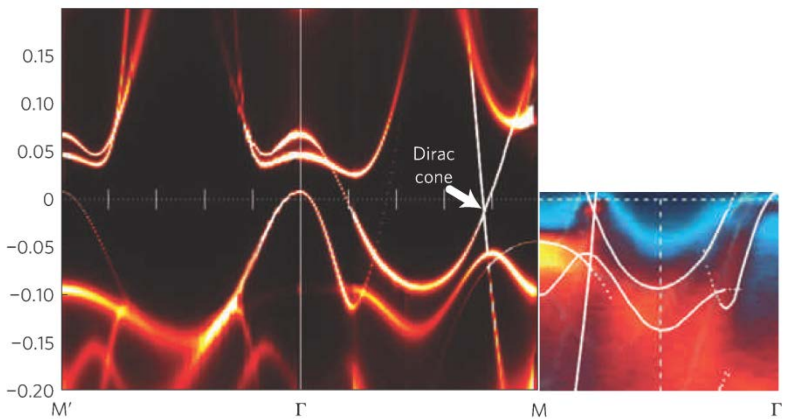
$$\sigma_{2,D}(\omega) = \frac{\sigma_0\omega\tau_D}{1+\omega^2\tau_D^2}$$

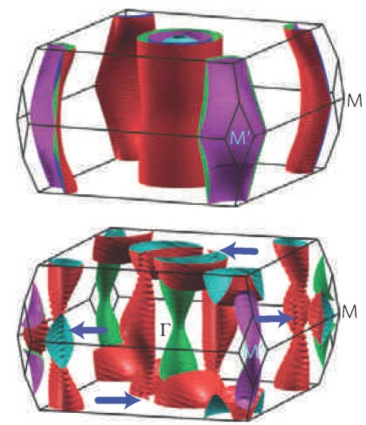


Y. M. Dai, CCH *et al.*, PRB **94**, 195142 (2016)

Fermi surface reconstruction

- Below T_N, Fermi surface reconstruction

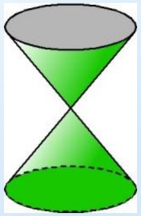




$T>T_N$

$T<T_N$

- Peaks in MIR arise from inter-band transitions
  - flat bands around Γ and M′ points
- ARPES, DFT+DMFT: <u>Dirac-like cones</u> below T_N
  - responsible for small scattering rate?



P. Richard *et al.,* Phys. Rev. Lett. **104**, 137001 (2010)
Z. P. Yin *et al*., Nat. Phys. **7**, 294 (2011)

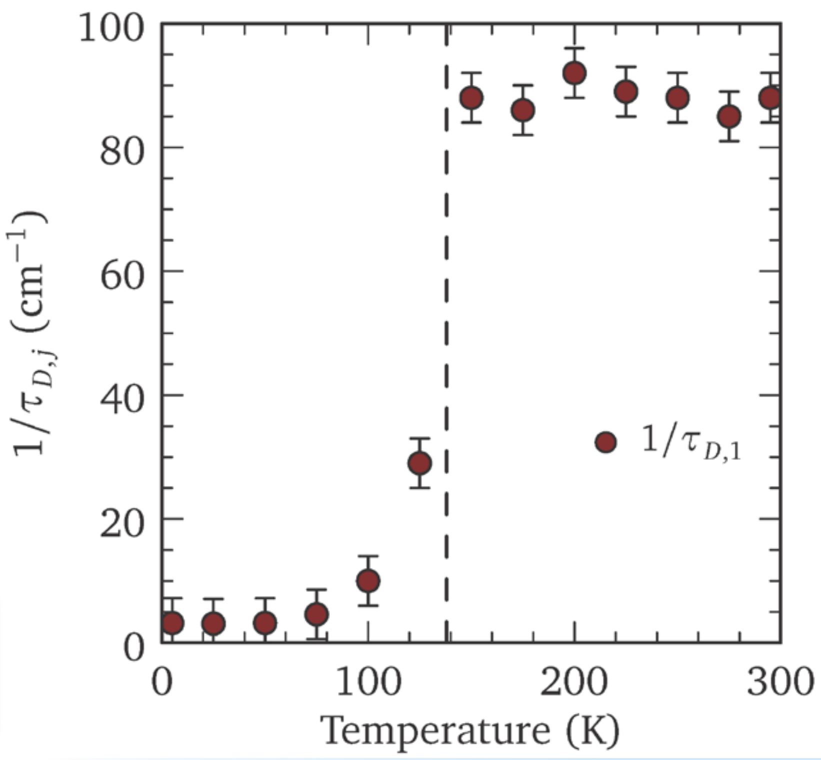
Scattering in semimetals

- Collapse of $1/\tau_{D,1}$ below T_N

$$1/\tau_{imp} \propto N(0)\,\varepsilon_F^2$$

- Fermi surface reconstruction below T_N:
  - Dirac-like cones: semimetal
  - decrease in the scattering rate of the coherent band likely the result of the reduction of the density of states at ε_F

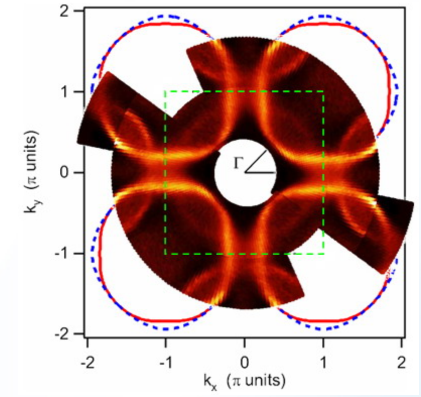
$BaFe_2As_2$

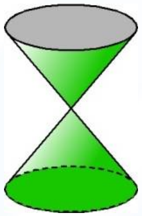


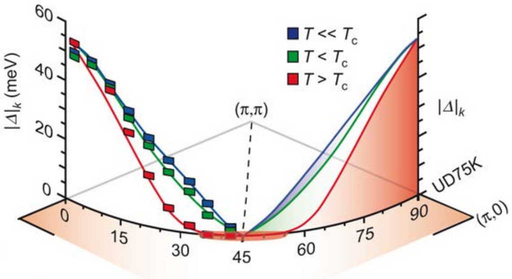
Y. M. Dai, CCH *et al.*, PRB **94**, 195142 (2016)

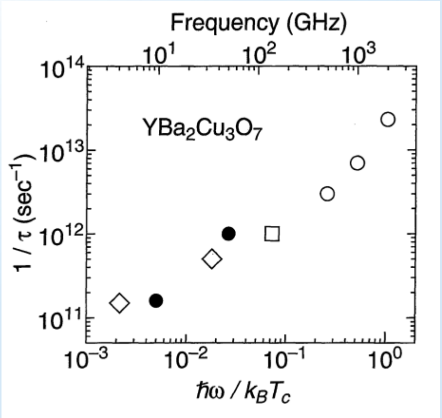
Cuprates

- Cuprates differ from the pnictides
  - single band vs multiband, etc.
- Optimal, overdoped materials:
  - large Fermi surface
- Underdoped: pseudogap
  - reduction in Fermi surface above T_c
- Below T_c: *d*-wave gap with nodes
  - unpaired quasiparticles at the nodes
  - nodes resemble Dirac cones
  - scattering rate collapses below T_c
    - similar to what is observed in pnictides below T_N







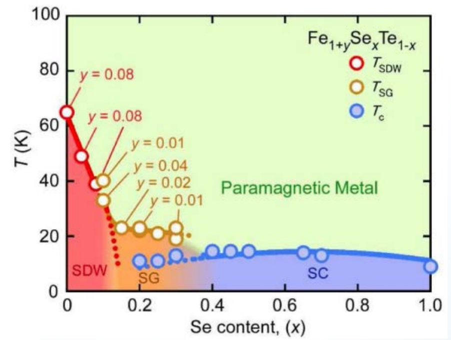


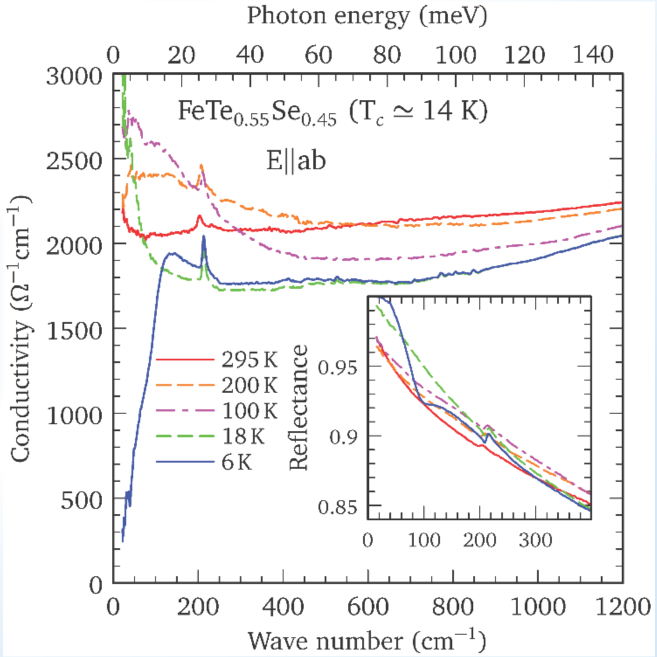
W. S. Lee *et al*., Nature **450**, 81 (2007)
T. Shibauchi *et al*., J. Phys. Soc. Jpn. **65**, 3266 (1996)
CCH *et al*., Sci. Rep. **3**, 3446 (2013)

Iron-chalcogenide superconductor

- FeSe (“11”) crystal: T_c~8 K

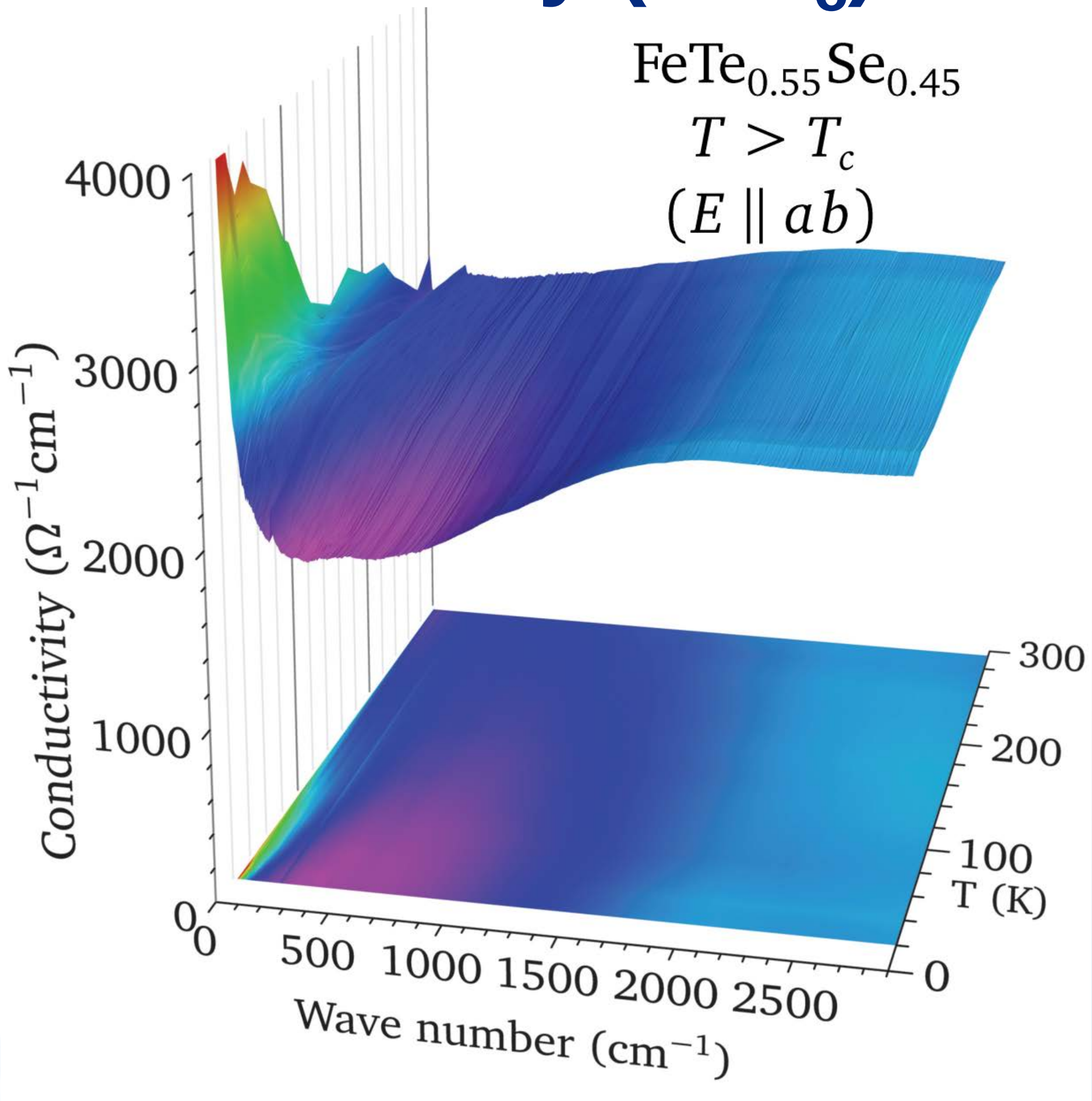
  (T_c is higher in thin films)
  - Te → Se nearly doubles T_c
- $FeTe_{0.55}Se_{0.45}$: T_c~14 K
- RT: almost incoherent response
  - Broad electronic background
  - Drude-like component narrows rapidly at low temperature
- Original work was limited…
  - did not consider multiband effects
  - no detailed temperature dependence below 100 K…





CCH *et al.*, Phys. Rev. B **81**, 180508(R) (2010)

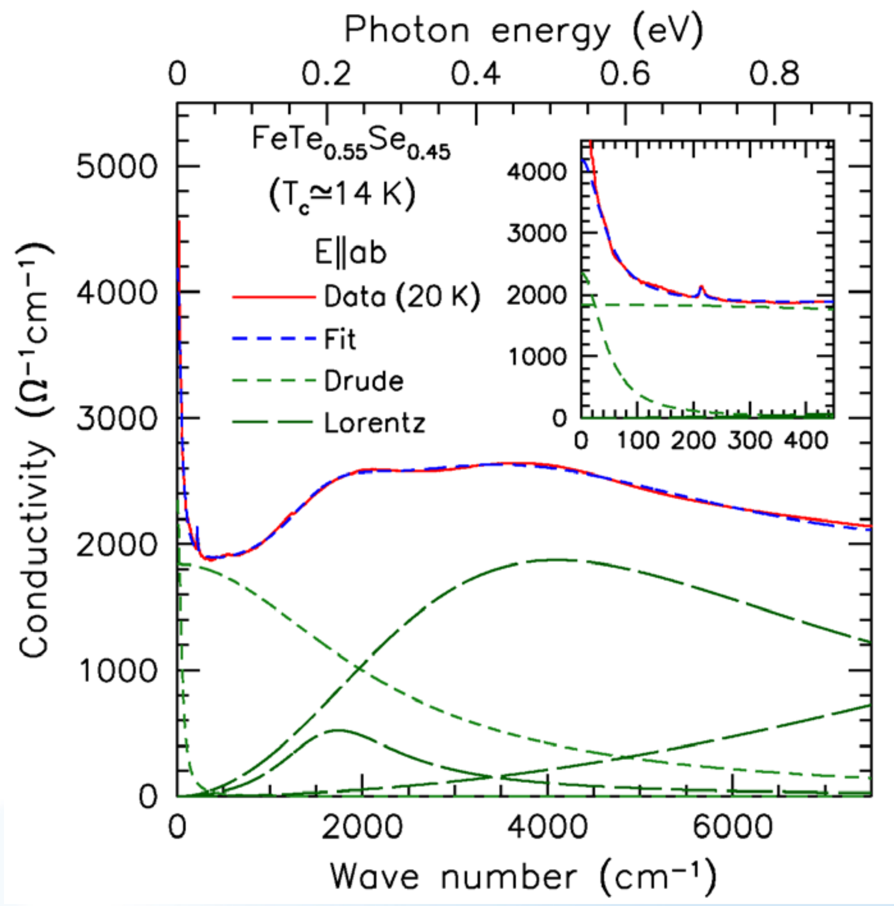
Optical conductivity ($T>T_c$): detail



CCH, Y. M. Dai *et al*., Phys. Rev. B **91**, 144503 (2015)

Model fits

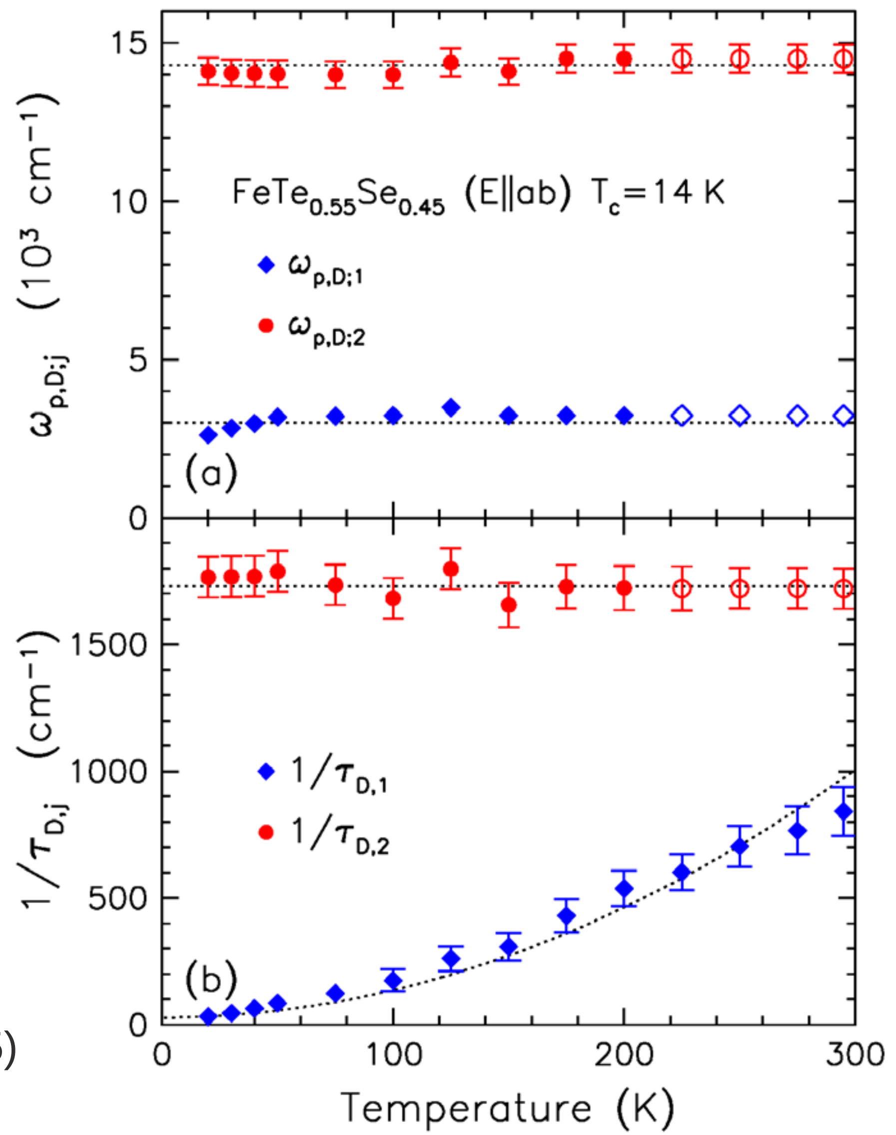
- $FeTe_{0.55}Se_{0.45}$
  - single Drude?
    - requires very low interband transition (~ 1 meV)
    - onset above 30 meV
- Two Drude model
  - strong, broad Drude
  - weaker, narrow
- $T \sim T_c$
  - Scattering rate for narrow Drude term has collapsed dramatically



D. Wu *et al*., Phys. Rev. B **81**, 100512(R) (2010)
B. Valenzuela *et al*., Phys. Rev. B **87**, 075136 (2013)
CCH, Y. M. Dai *et al*., Phys. Rev. B **91**, 144503 (2015)

Drude parameters – scattering rates

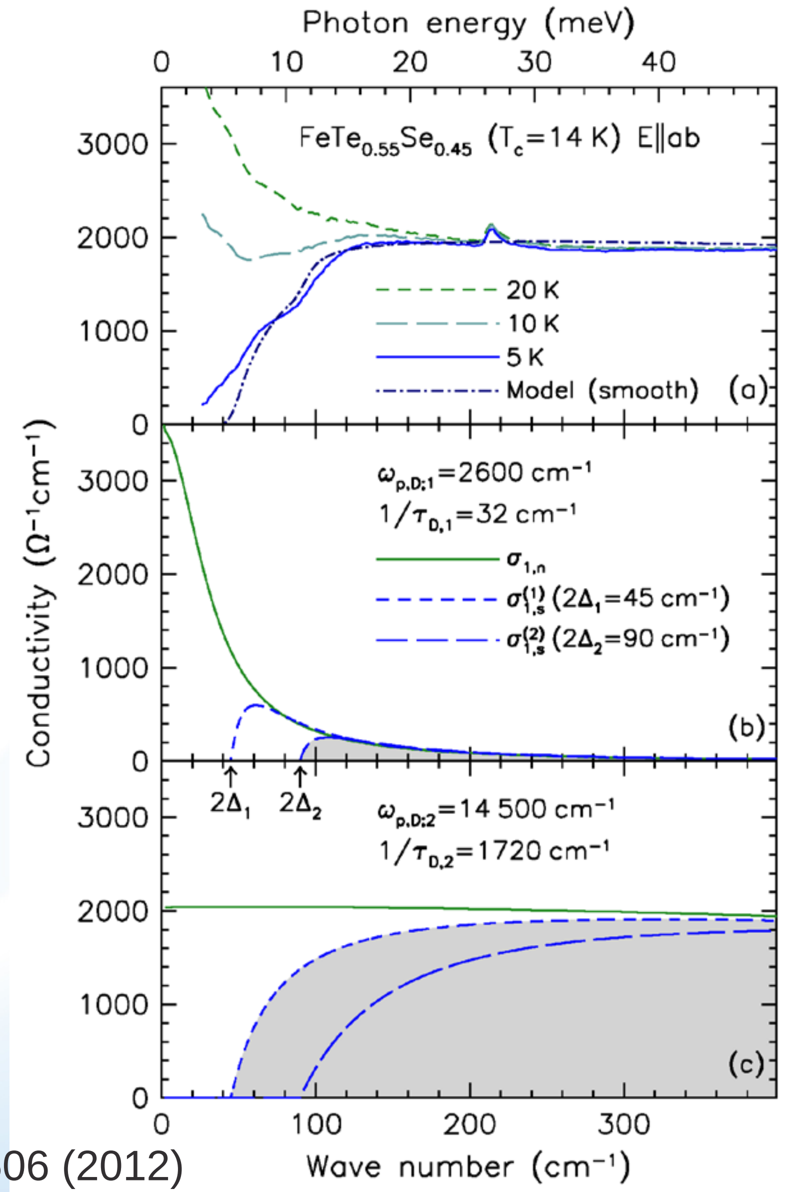
- Strong, broad Drude:
  - little temperature dependence
- Weaker, narrow Drude:
  - Strength doesn't vary
  - Scattering rate strongly temperature dependent
    - dominates transport at low temperature
- Hidden Fermi liquid?
  - $1/\tau_{D,1}$ quadratic with T?



CCH, YMD *et al.*, Phys. Rev. B **91**, 144503 (2015)

$FeTe_{0.55}Se_{0.45}$: multiband SC

- Multiple bands, multiple gaps
  - Δ_1~2.8 meV, ($2\Delta_1$~45 cm^{-1})
  - Δ_2~5.6 meV, ($2\Delta_2$~90 cm^{-1})
- Weak Drude ($1/\tau_1$~4 meV)
  - $1/\tau_1 < 2\Delta_{1,2}$: approaching clean limit
- Strong Drude ($1/\tau_2$~215 meV)
  - $1/\tau_2 >> 2\Delta_{1,2}$: dirty limit
- Mattis-Bardeen modeling
  - large gap: weak Drude
  - small gap: strong Drude
    - works well, no refinement!
- ARPES: large gap associated with electron pocket



H. Miao *et al*., Phys. Rev. B **85**, 094506 (2012)

Superfluid density

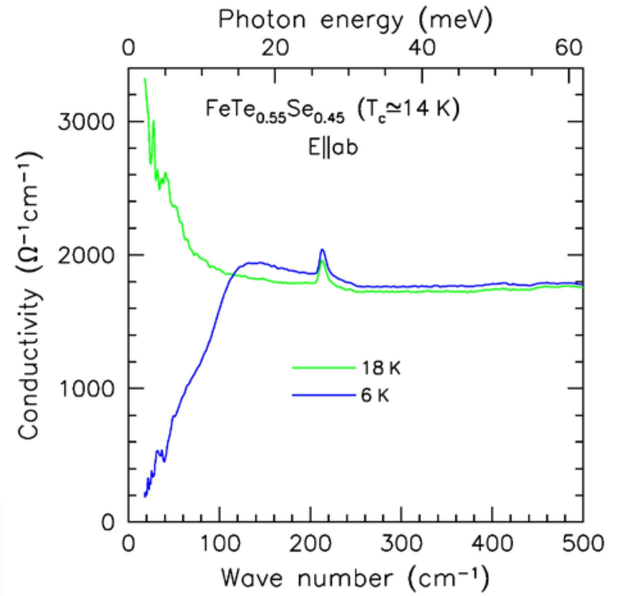
- Ferrell-Glover-Tinkham sum rule
  - works for multiband materials
  - energy scale for SC ~ 12 meV
    - consistent with estimate for gaps

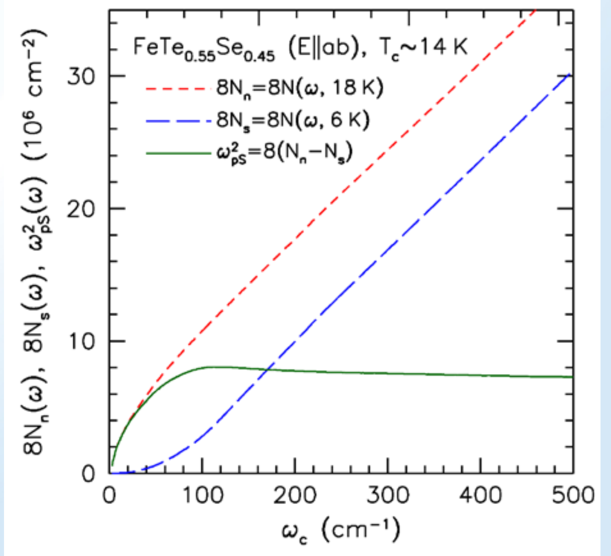
$$\int_{0^+}^{\omega_c}\left[\sigma_1(\omega, T \cong T_c) - \sigma_1(\omega, T \ll T_c)\right] d\omega = \frac{\omega_{p,S}^2}{8}$$

$$\boxed{\begin{array}{c} \omega_{p,S} \cong 3280 \pm 300\ \mathrm{cm}^{-1} \\ \lambda_0 \cong 490 \pm 20\,\mathrm{nm} \end{array}}$$

- Mattis-Bardeen model

$$\boxed{\begin{array}{c} \omega_{p,S;1} \cong 2300\ \mathrm{cm}^{-1},\ \omega_{p,S;2} \cong 2740\ \mathrm{cm}^{-1} \\ \omega_{p,S} = \sqrt{\omega_{p,S;1}^2 + \omega_{p,S;2}^2} \\ \omega_{p,S} \cong 3750\ \mathrm{cm}^{-1} \end{array}}$$





Scaling of the superfluid density

- Empirical scaling relation

$$\rho_{s0}/8 \cong 4.4\,\sigma_{dc} T_c$$

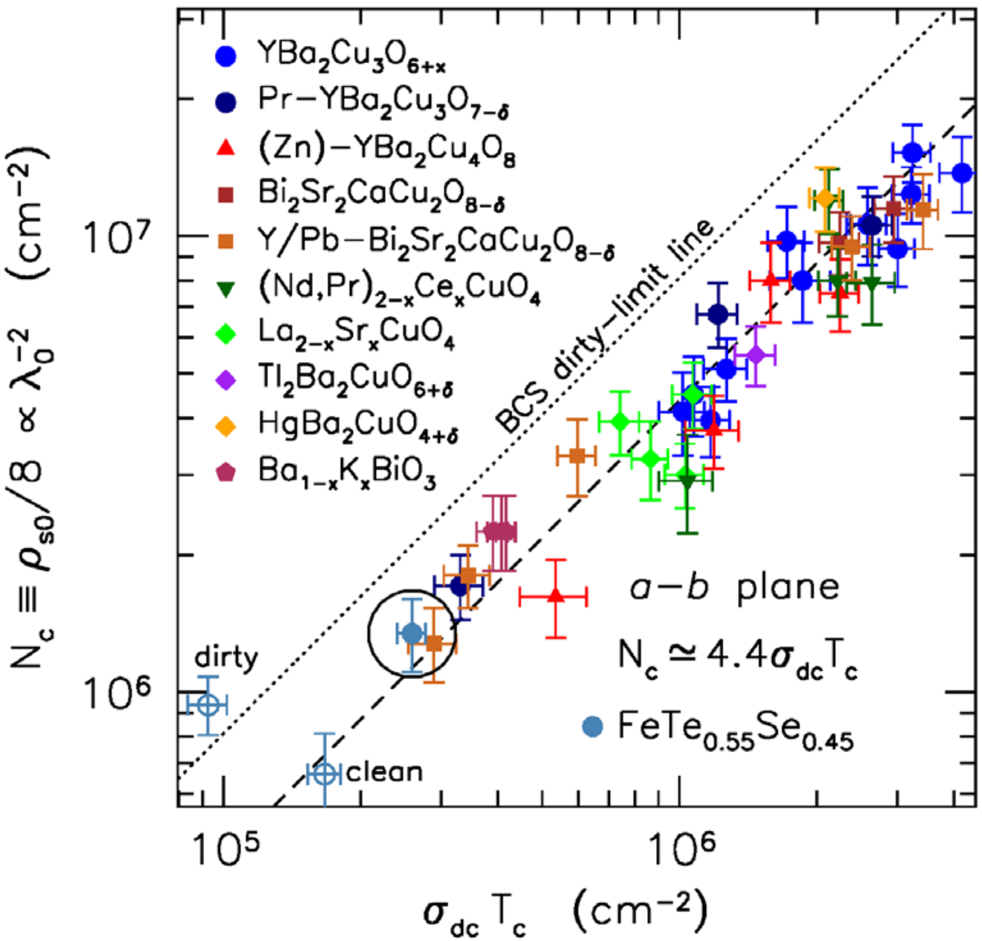
- Narrow Drude

$$\boxed{\begin{array}{c} \sigma_{dc,c} \cong 3600\,\Omega^{-1}\mathrm{cm}^{-1} \\ \omega_{pS,c} \cong 2300\,\mathrm{cm}^{-1} \end{array}}$$

  - clean limit
- Broad Drude

$$\boxed{\begin{array}{c} \sigma_{dc,c} \cong 2000\,\Omega^{-1}\mathrm{cm}^{-1} \\ \omega_{pS,c} \cong 2740\,\mathrm{cm}^{-1} \end{array}}$$

  - dirty limit
  - agrees with BCS prediction
- Total: falls on scaling line



CCH *et al.,* Nature **430**, 539 (2004); Phys. Rev. B **72**, 134517 (2005)
V. G. Kogan, Phys. Rev. B **87**, 220507(R) (2013)

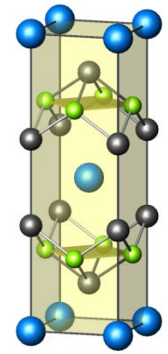
$FeTe_{0.55}Se_{0.45}$

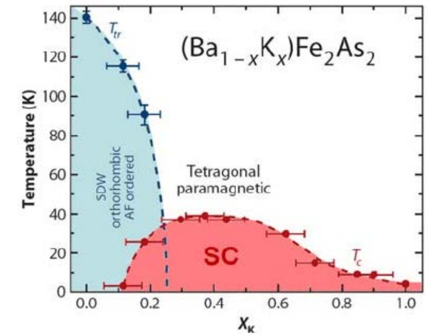
- Normal state:
  - two-Drude model describes the optical conductivity very well
- Superconducting state:
  - multiple bands, multiple gaps
  - Mattis-Bardeen dirty limit approach
  - simultaneously in the clean and dirty limit!
  - falls on scaling line
- In the two-Drude approach, the coherent band narrows considerably (RT $\rightarrow$ 20 K, 840 $\rightarrow$ 30 cm^{-1})
  - hidden Fermi liquid behavior?
  - observed in other iron-based materials?

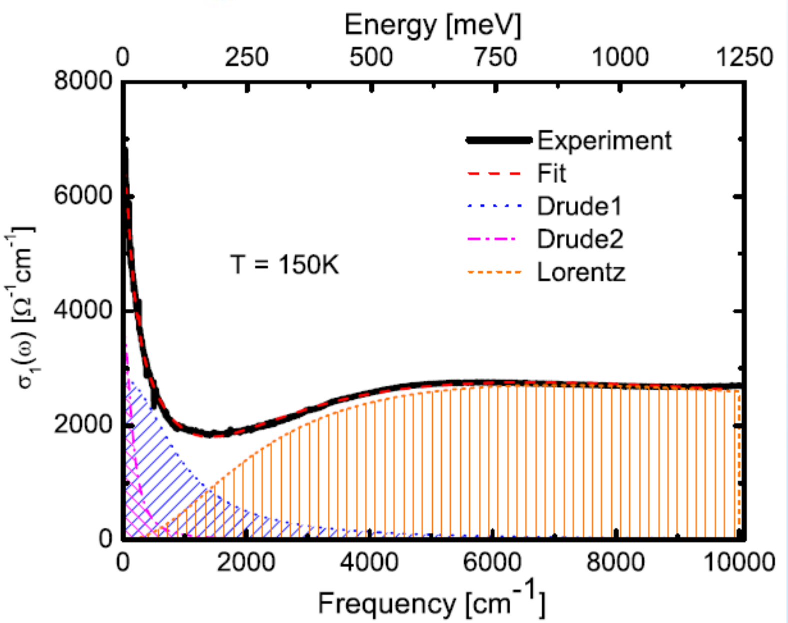
CCH, Y. M. Dai *et al*., Phys. Rev. B **91**, 144503 (2015)
Y. M. Dai, CCH *et al.*, Phys. Rev. B **93**, 054508 (2016)

$Ba_{0.6}K_{0.4}Fe_2As_2$

- K-doped $BaFe_2As_2$
  - hole doped
  - SC over broad doping range
- $Ba_{0.6}K_{0.4}Fe_2As_2$ (T_c~39 K)
  - $T>T_c$: 12 temperatures
- Fit with two-Drude model
  - strong, broad term
  - weaker, narrow term
- T-dependence
  - plasma frequencies
  - scattering rates



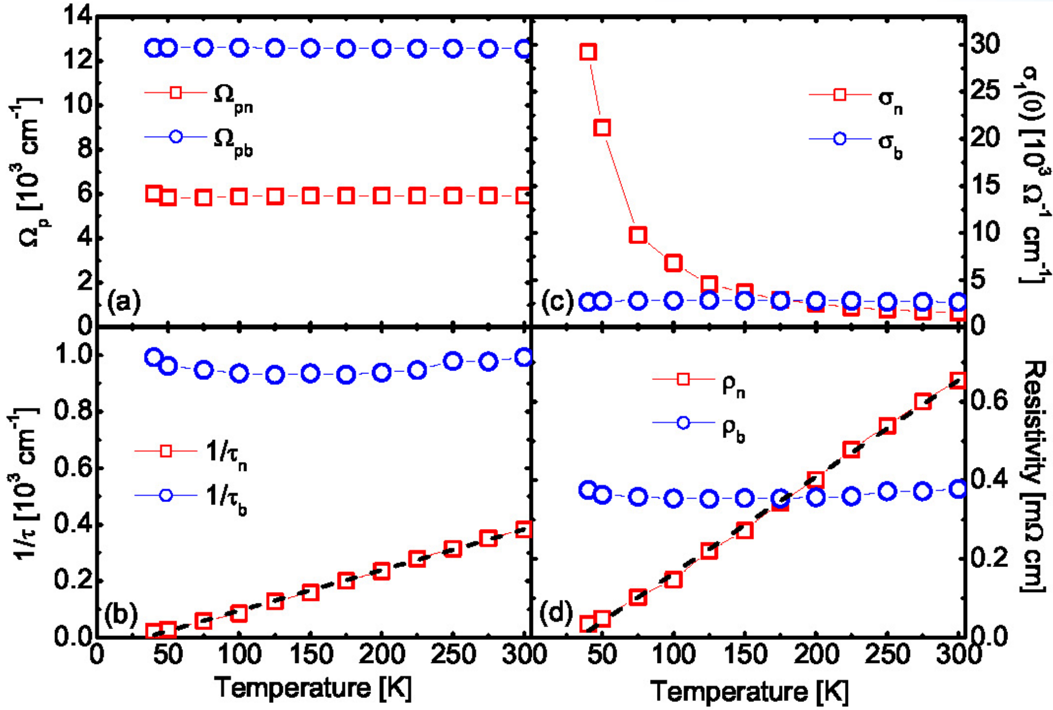




Y.M. Dai *et al.*, Phys. Rev. Lett. **111**, 117001 (2013)

$Ba_{0.6}K_{0.4}Fe_2As_2$: hidden non-FL behavior

- Drude $\omega_{p,D}$: constant
  - carrier concentration in pockets not changing
- Strong term: $1/\tau$ constant
- Weak term: $1/\tau \propto T$!
  - non-Fermi liquid
  - dramatic decrease in $1/\tau$
    - $1/\tau \sim 20\ cm^{-1}$ at 40 K
- Calculate contribution to resistivity from each pocket
  - crossover at ~ 170 K
  - observed in transport



Y.M. Dai *et al.*, Phys. Rev. Lett. **111**, 117001 (2013)

Summary

- Iron-based materials: multiband (*e* and *h* pockets)
  - two-Drude model required
- $BaFe_2As_2$: broad, narrow Drude components
  - collapse of scattering rate connected to Fermi surface reconstruction, Dirac-like cones
  - Dirac & Weyl semimetals: small scattering rates
    - due to small density of states at Fermi level
    - analogous behavior in cuprates below T_c?
- $FeTe_{0.55}Se_{0.45}$ (T_c~14 K) & $Ba_{0.6}K_{0.4}Fe_2As_2$ (T_c~39 K)
  - multiple bands & gaps; Fermi liquid and non-Fermi liquid
  - in both the clean and dirty limit – true for all iron-based SC's?
  - iron-based superconductors follow universal scaling law